Title:	Parallel Simulation of Beam Dynamics in Particle Accelerators
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Intended for:	Report
Issued:	2021-03-25

Parallel Simulation of Beam Dynamics in Particle Accelerators

LANL Institutional Computing Project w20_accelsim

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March 22, 2021

Outline

- 2-slide summary
- Full presentation
  - Overview of the parallel Lienard-Wiechert (LW) code, LW3D
  - Application to modeling undulator radiation
  - Self-consistent N-body dynamics with radiation

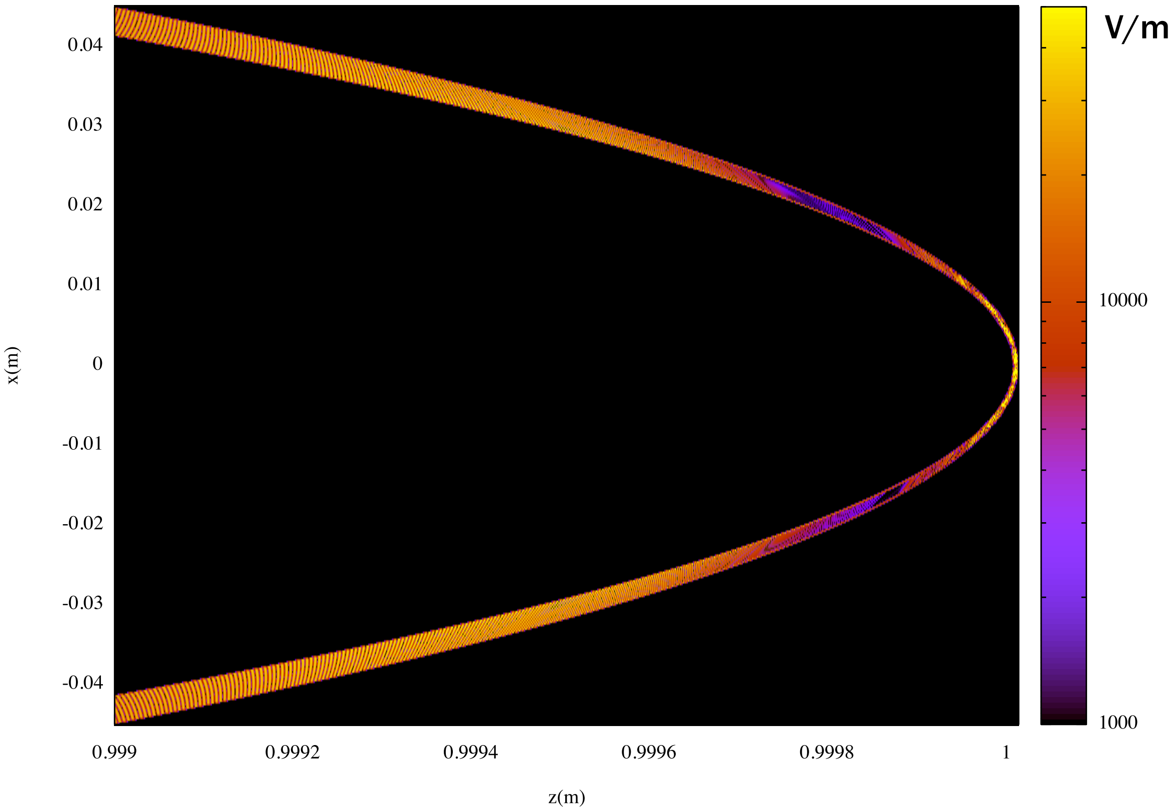
Project w20_accelsim goals, accomplishments, plans

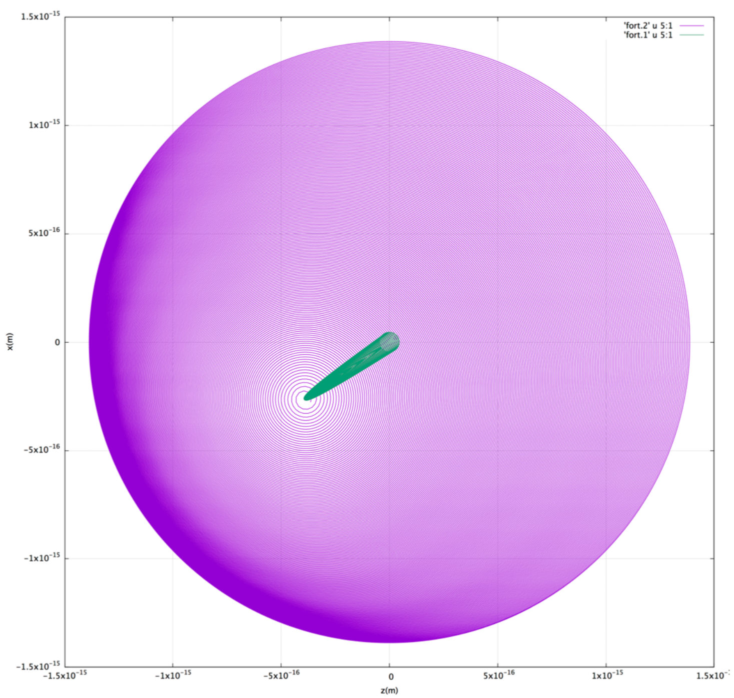
- Develop and apply parallel beam dynamics capabilities that are relevant to LANL programs
  - Undulator-based, non-invasive current profile diagnostic that is being developed under LANL LDRD project 20190294ER
  - Other LANL programs involving high brightness electron beams

- Accomplishments
  - Lienard-Wiechert 3D code (LW3D) modified to simulate undulator radiation
  - LW3D code is installed on Capulin @ LANL and Cori @ NERSC
    - Performance example: A simulation on 9000 cores of Capulin using 1M electrons takes < 5 minutes to compute the LW fields at 20K observation points
  - Simulations performed to prediction classical undulator radiation from a large number of electrons from first principles.
  - Self-consistent N-body version of LW3D tested on the electrodynamic 2-body problem. Results in agreement with theory.

- Plans
  - LW3D will be used to test an analytical model of undulator radiation that was developed under the LDRD project
  - Enhance LW3D to study self-consistent radiative effects in beam manipulation systems like chicanes

Sample results





LW3D simulation of undulator radiation performed on Capulin. The plot shows the magnitude of the transverse electric field downstream from the undulator. On the right side of the plot near the axis (x=0) the radiation is incoherent. On the left side off-axis, the narrow dark/light bands denote coherent radiation.

Capulin simulation of two particles spiraling in toward one another as they radiate and interact via retarded Lienard-Wiechert fields.

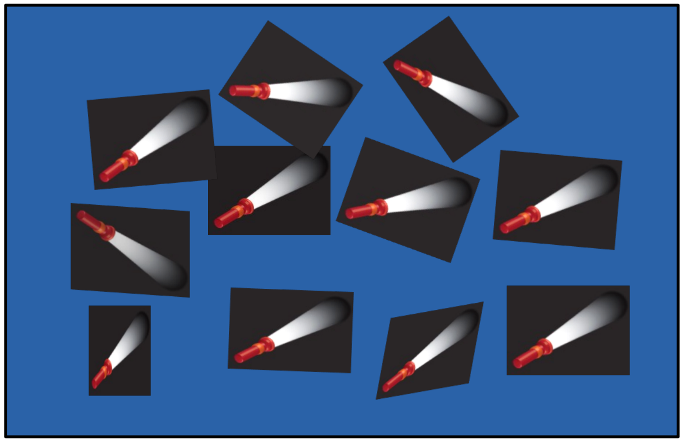
Full Presentation:
Introduction

- Space-charge effects in intense beams have been studied for decades
  - Important in high intensity proton beams, low energy electron beams
  - Significant focus at LANL in past – PARMILA, PARMELA, beam halo,…
  - First 3D parallel space-charge codes* developed at LANL/ACL in 1990's
    - Since then 3D space-charge codes have sprung up worldwide
- Despite major advances in space-charge modeling, there is still no 3D code that can efficiently model 3D radiative effects like coherent synchrotron radiation (CSR) and be used for design
  - Key factor affecting quality of high brightness electron beams in FELs
- Why is modeling 3D radiative phenomena so difficult???

* "space charge code" = electrostatic-in-beam-frame PIC code

Exploring synchrotron radiation through simulation is extremely challenging

- Synchrotron radiation: arguably the least well modeled physical phenomenon in e- linacs for future light sources
  - Most codes use a simplified 1D model
- Highly important to beam quality and beam stability
  - Damages beam quality; radiation from the tail takes a shorter path than the beam in a bending magnet, can disrupt the front of the bunch
- Challenging spatial/temporal dependence: radiation in a tiny cone angle along with retardation effects
  - Imagine a billion ultra-narrow flashlight beams shining on and interacting with each other



Overview of the LW3D Code

LW3D is an outgrowth of a code originally developed under a LANL LDRD project, *Exploiting Hamiltonian Properties of Beams to Revolutionize X-Ray Free-Electron Laser Architectures*, led by Bruce Carlsten, that included me (RDR) as an external collaborator

Initial development was aimed at predicting and studying 3D CSR

First version of the code used a “particle-to-grid” model (“given a set of particles and their histories, compute the field on a grid of observation points”)

A convolution-based model has also been developed.

Lienard-Wiechert Field

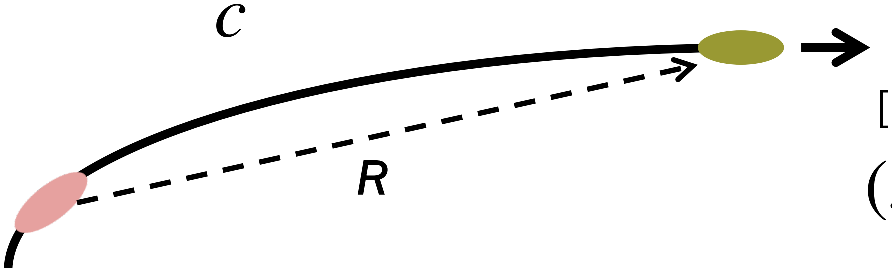
$$\boldsymbol{E} = \frac{1}{4\pi\varepsilon_0}\left[\frac{q}{\gamma^2\kappa^3 R^2}(\boldsymbol{n}-\boldsymbol{\beta}) + \frac{q}{\kappa^3 Rc}\boldsymbol{n}\times\left((\boldsymbol{n}-\boldsymbol{\beta})\times\frac{\partial\boldsymbol{\beta}}{\partial t}\right)\right]_{ret}$$

$$\boldsymbol{\beta} = \mathbf{v}/c$$

$$\boldsymbol{n} = \boldsymbol{R}/|\boldsymbol{R}|$$

$$\kappa = 1 - \boldsymbol{n}\cdot\boldsymbol{\beta}$$

$$\boldsymbol{B} = \frac{1}{c}\boldsymbol{n}\times\boldsymbol{E}$$



R points from the radiating particle's position at the retarded time to the observation point at the observation time

$[\ldots]_{ret}$ denotes quantities evaluated at the retarded time,

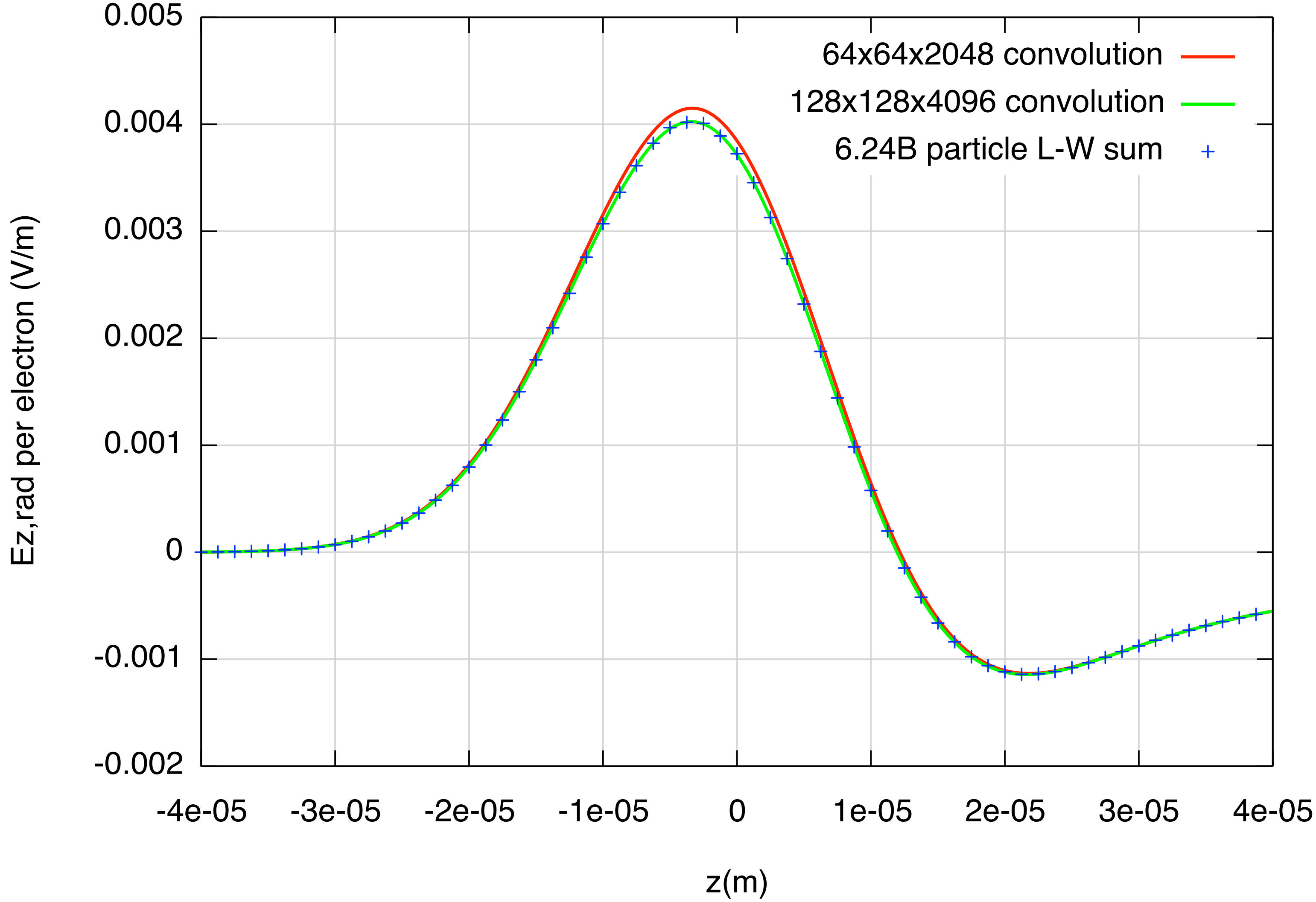
$$(x-x_r)^2 + (y-y_r)^2 + (z-z_r)^2 = c^2(t-t_r)^2$$

Light cone condition

Basic Code Components: Particle-to-Observation Point Solver

- Lorentz force integrator + storage of particles' histories
- Bisection search as first step to find retarded quantities
- Iterative solver as final step to find retarded quantities
- Computation of Lienard-Wiechert fields
- Parallelization with MPI
- Pitfalls/Issues:
  - Small step size → large memory
  - Large step → iterative solver more time-consuming
  - Care required to perform a high precision iterative search based on quantities determined by (imperfect) numerical integration
    - Situation exacerbated when the retarded position is close to the observation point due to pathological nature of LW Green's function

Example: Lienard-Wiechert simulation of steady-state dipole radiation

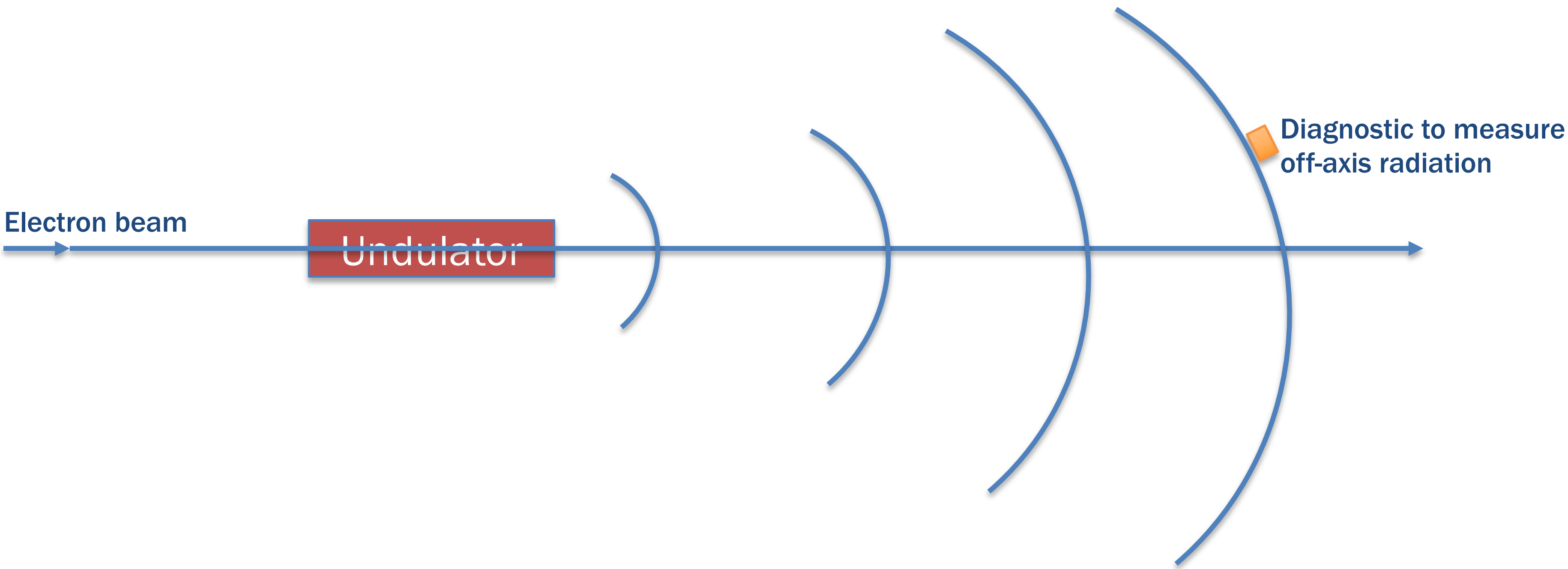


Modeling Undulator Radiation

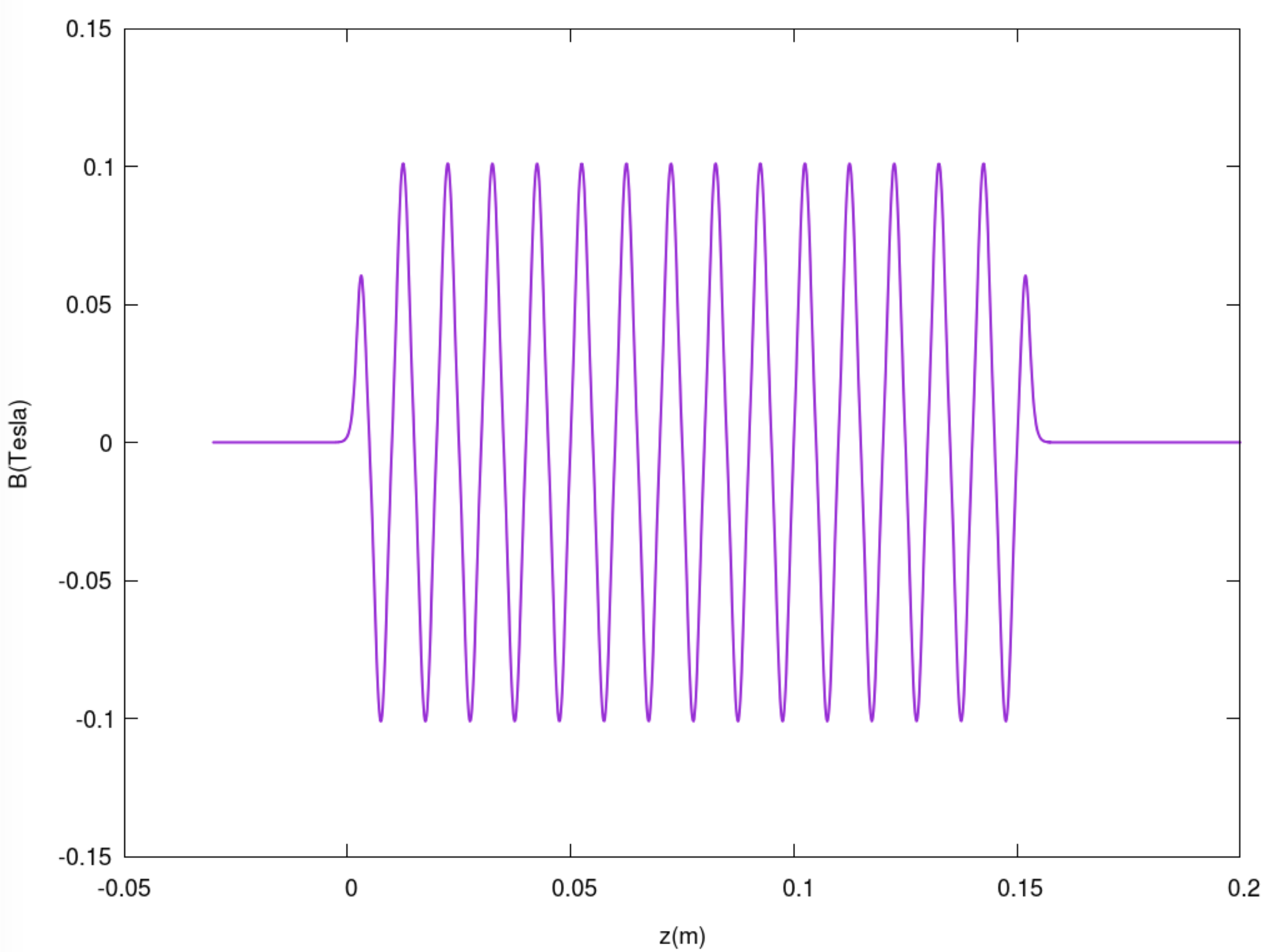
Recently LW3D was modified to be better suited to model undulator radiation

Motivation is a LANL LDRD to develop and test a non-invasive beam profile monitor.

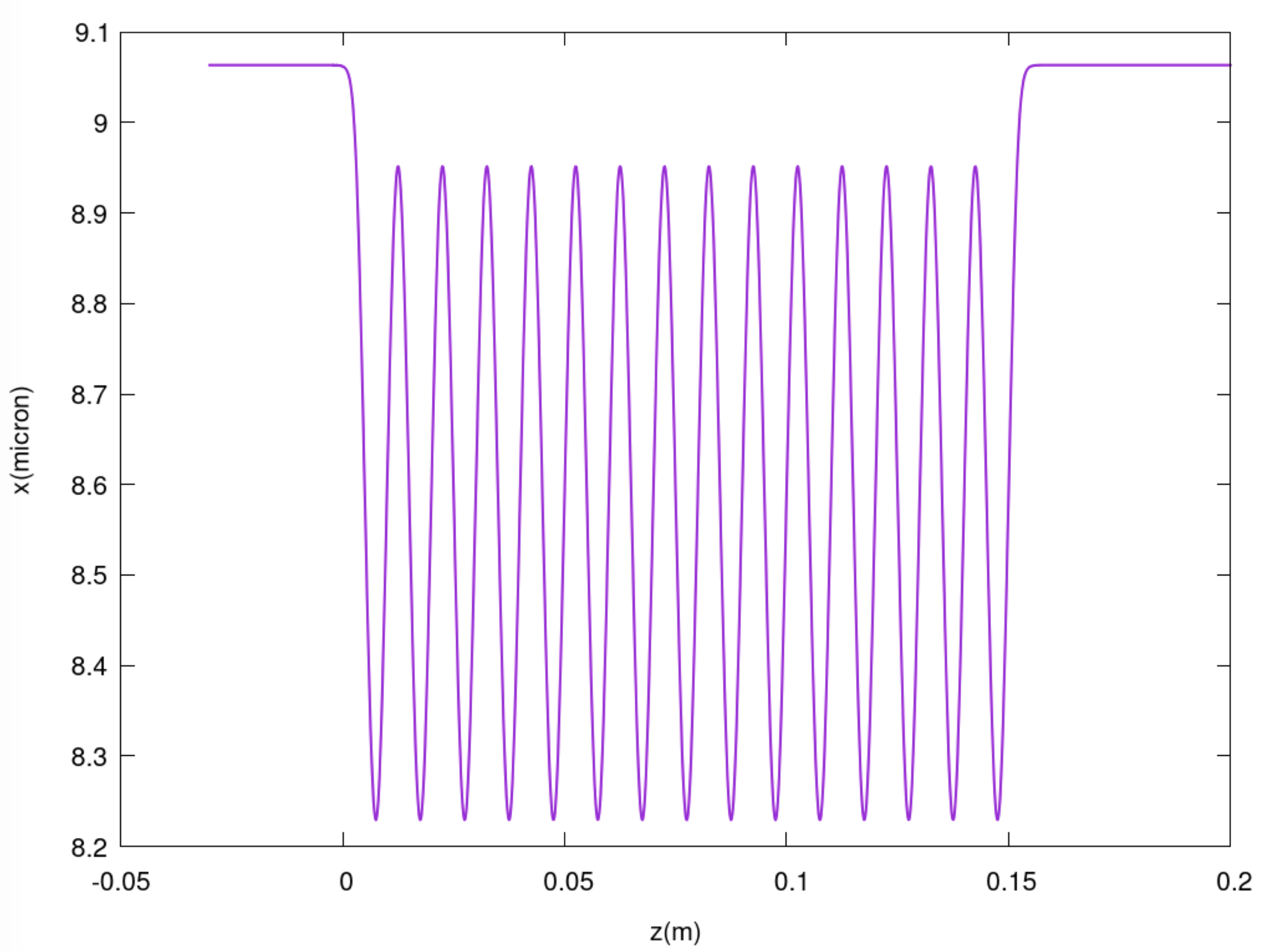
Example Setup
(drawing not to scale)



Undulator magnetic field profile

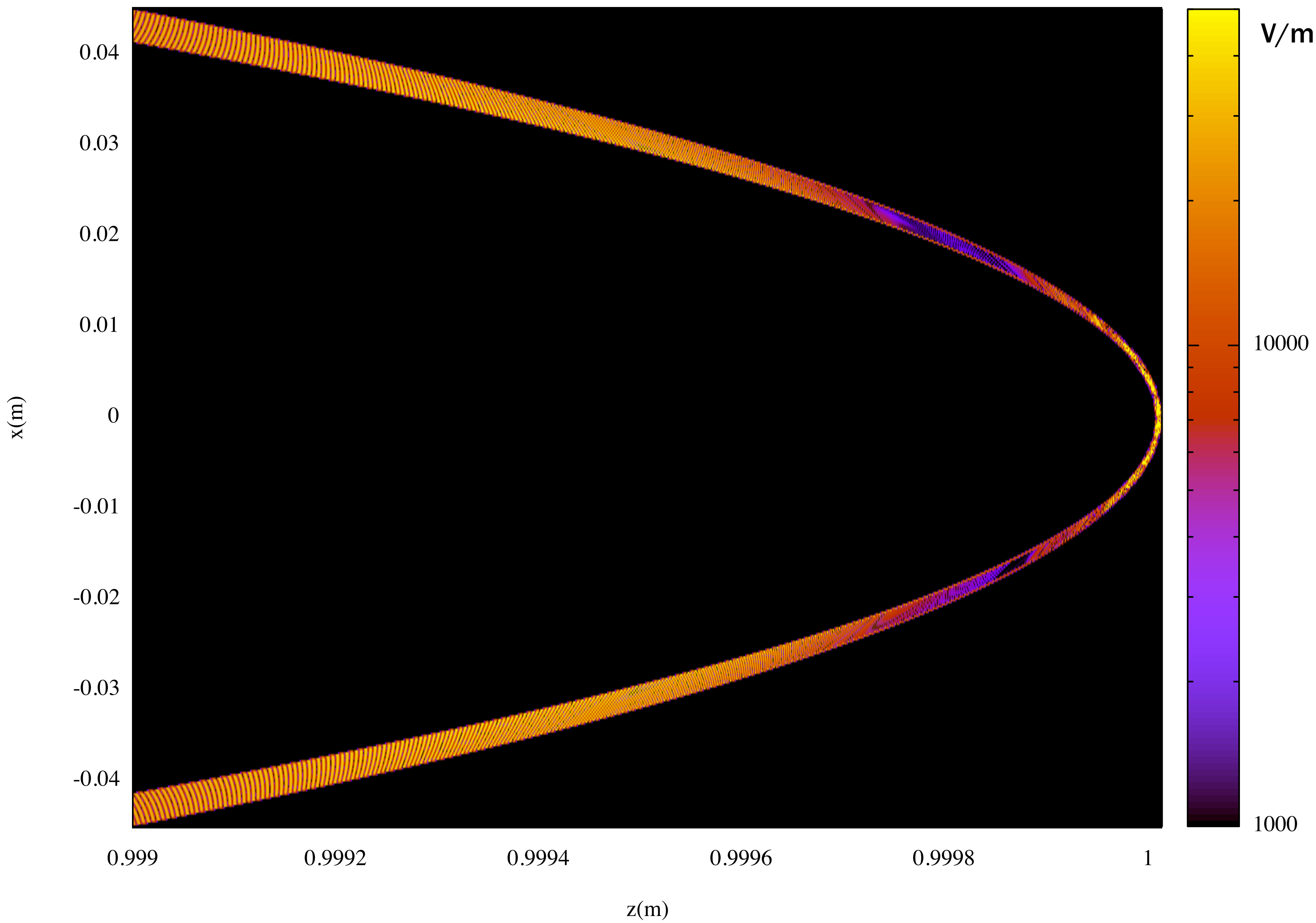


Electron trajectory inside the undulator



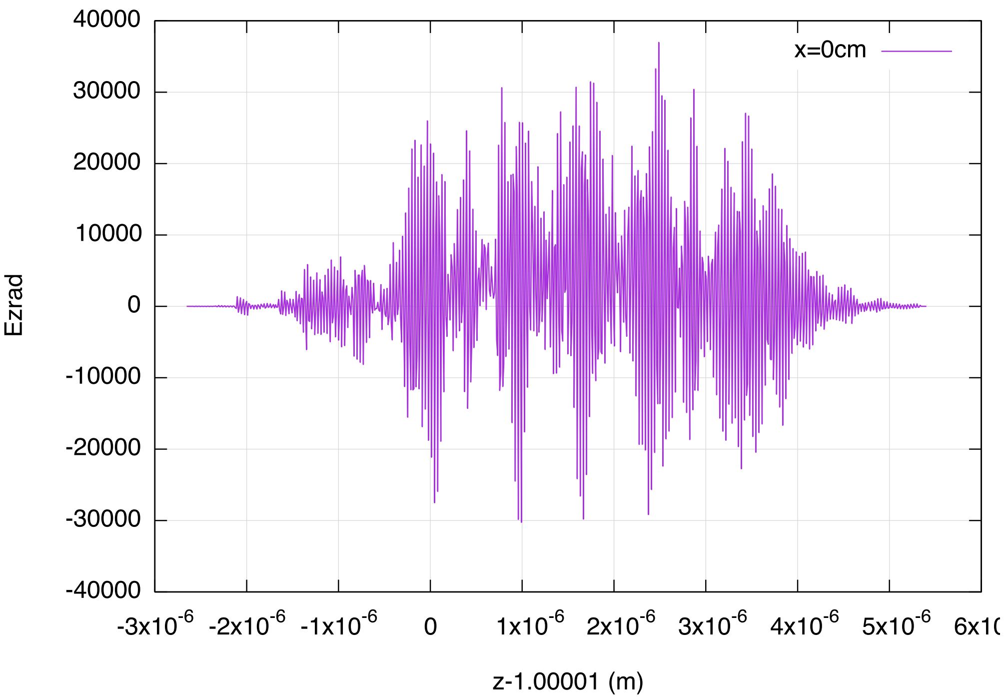
Plot of |Ez| in the x-z plane downstream of undulator

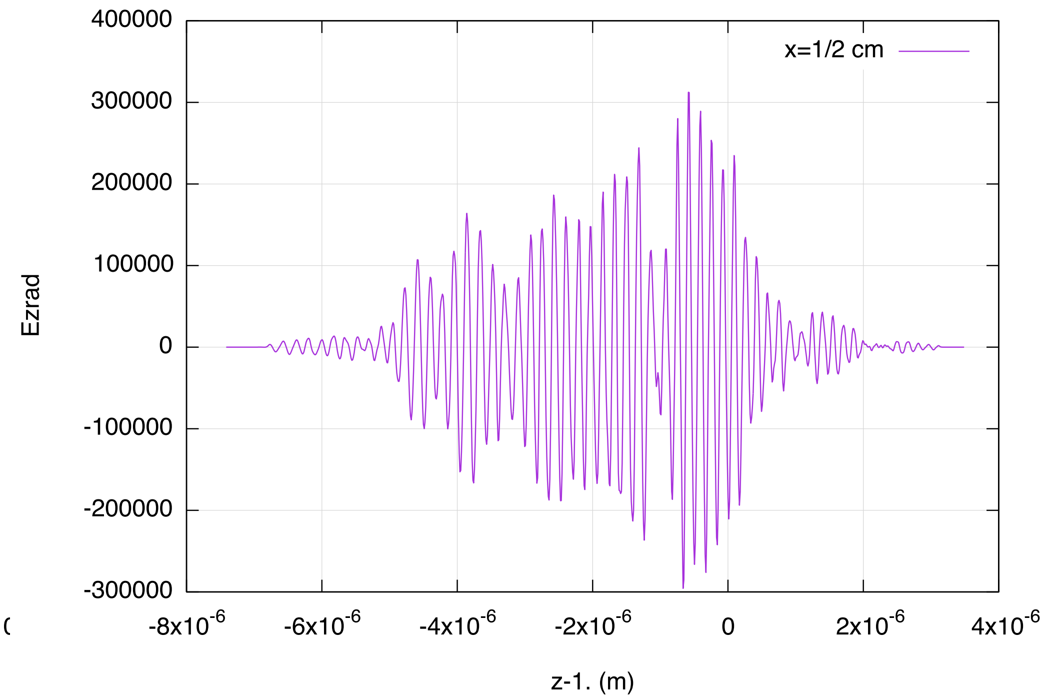
LW3D simulation of undulator radiation performed on Capulin



The simulation results exhibit both the coherent radiation and the incoherent radiation

Incoherent radiation on or near the axis





Lineout on axis

Lineout at x=0.5cm

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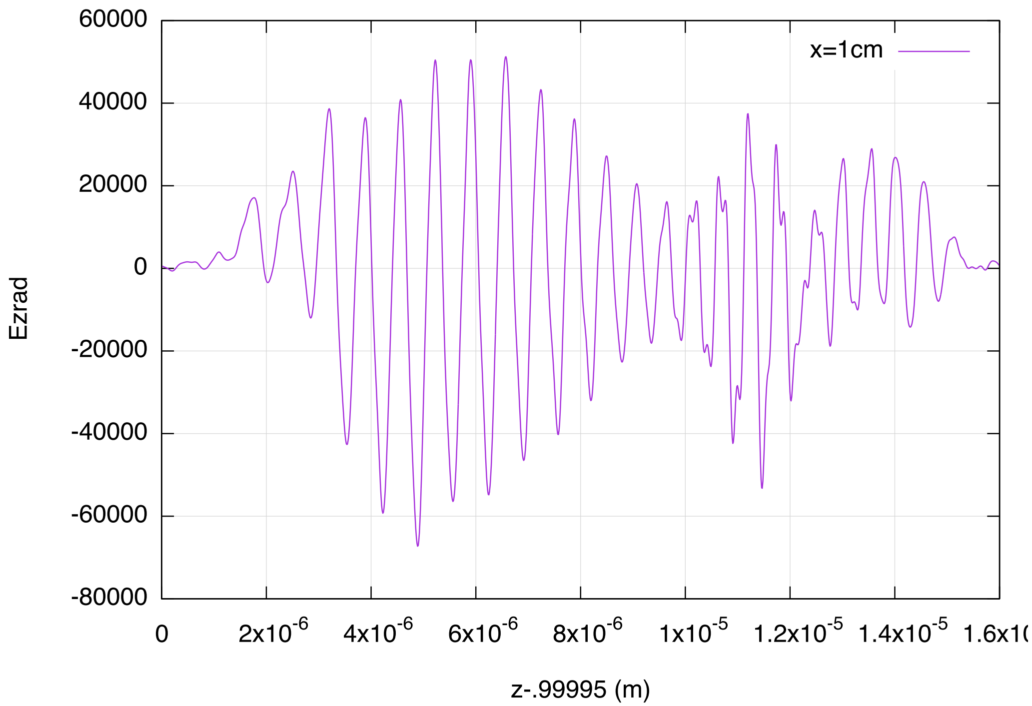
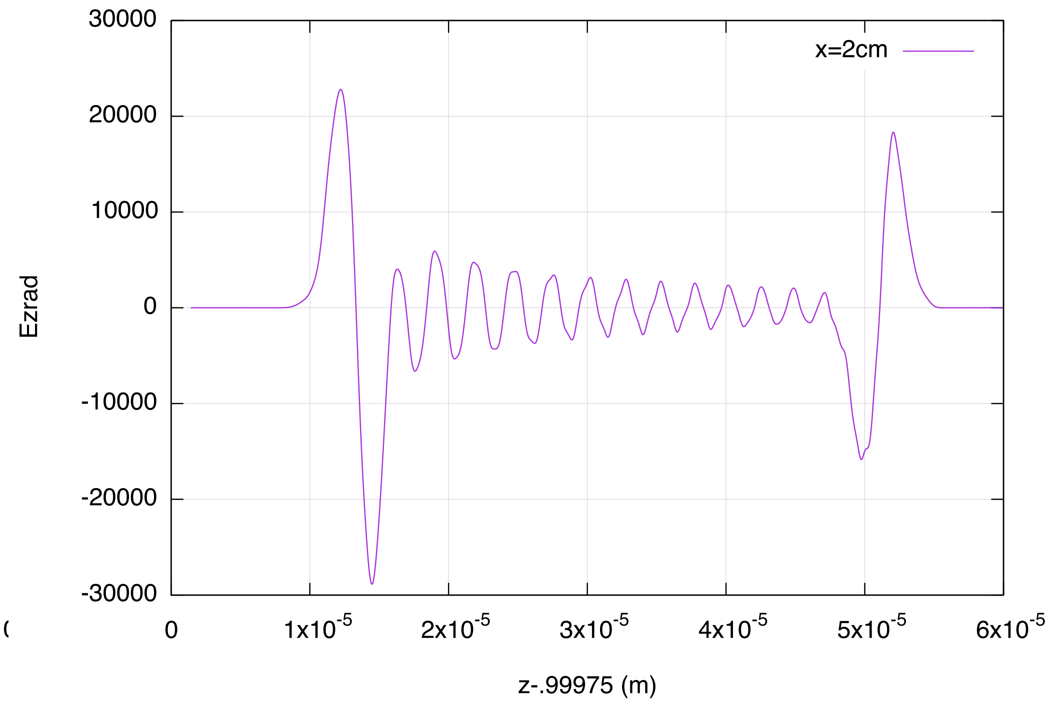
Incoherent signal is reduced, and coherent signal increases, moving away from the axis



Lineout at x=1cm



Lineout at x=2cm

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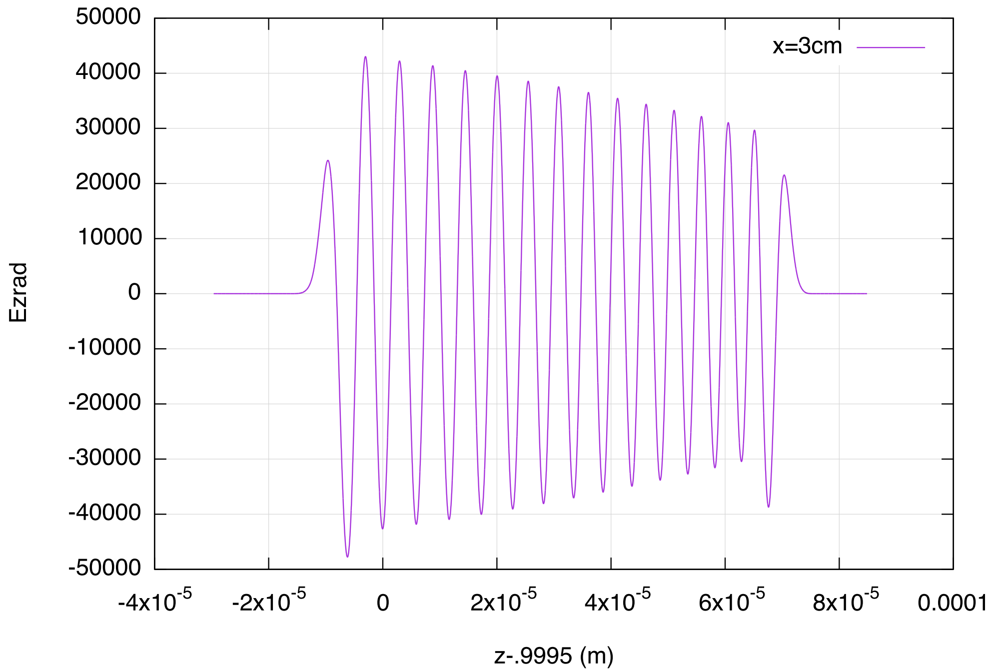
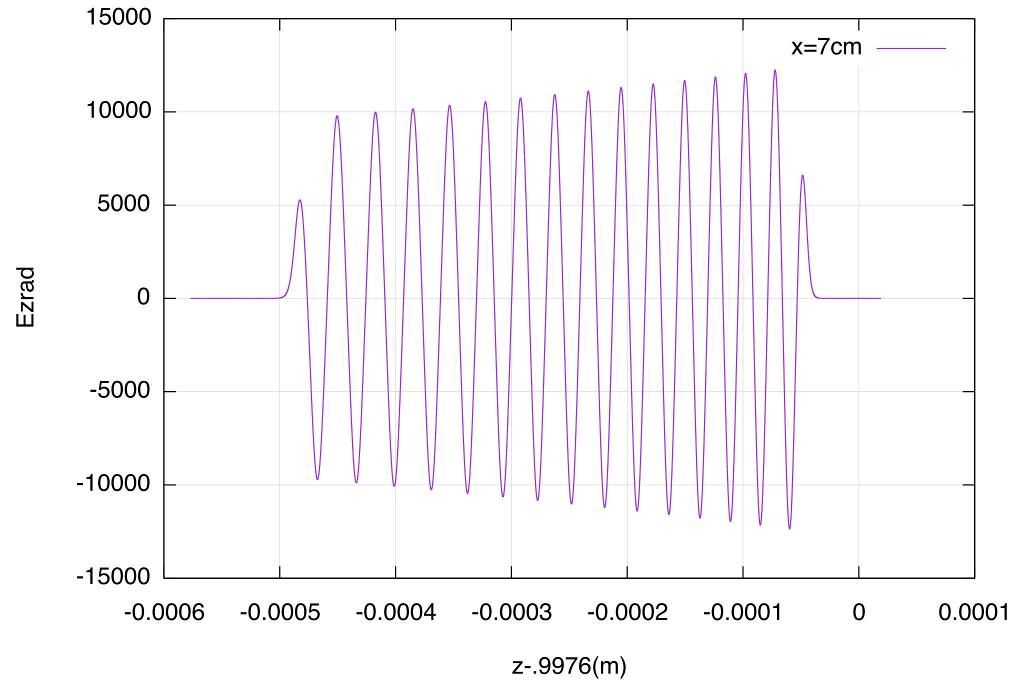
Coherent radiation off axis



Lineout at x=3cm



Lineout at x=7cm

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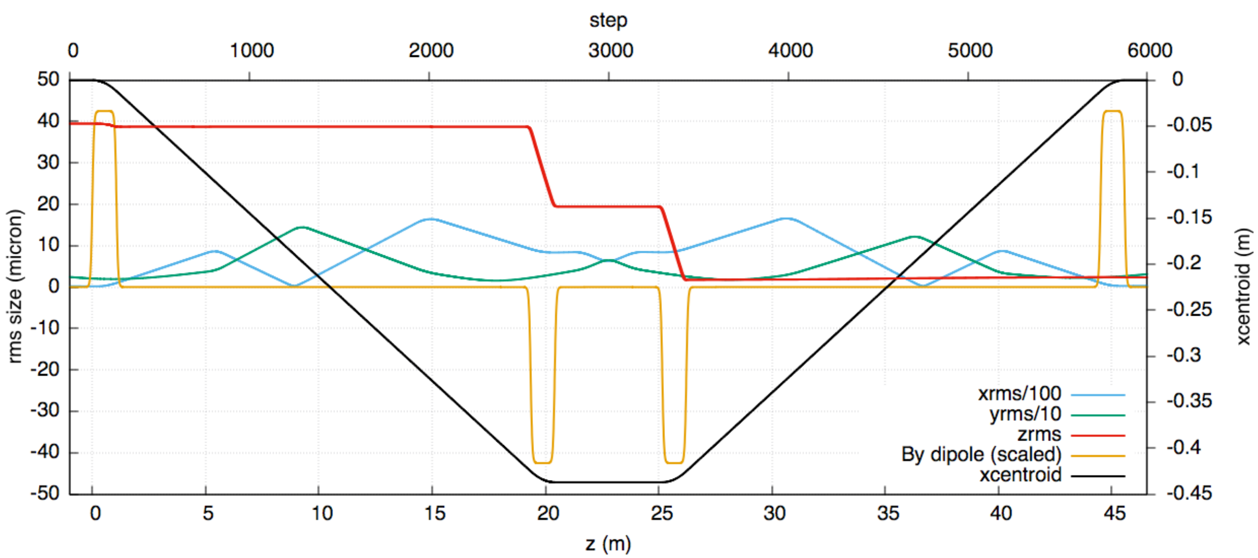
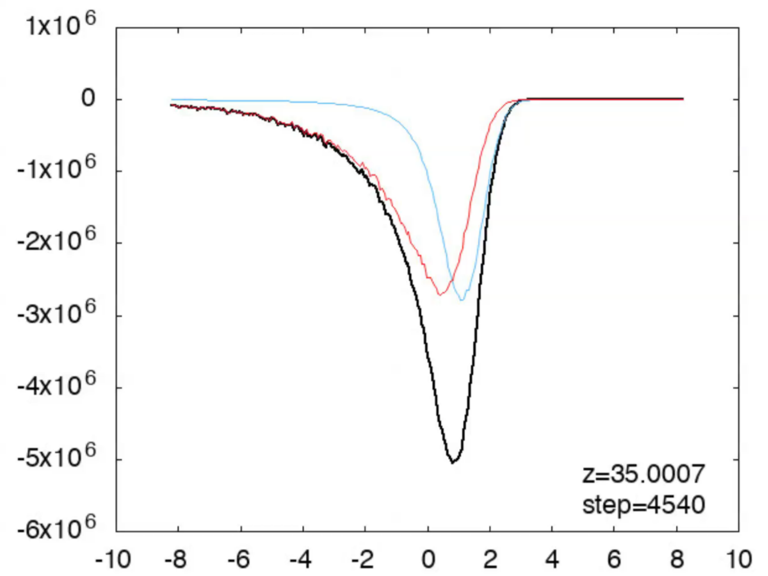
Modeling Coulomb and Radiative Self-Fields in Beam Manipulation Systems

- Example: Beam dynamics in a chicane for bunch compression
- Plot of rms envelopes (lower left) shows that the beam size is highly 3 dimensional.
- Movie of self-field (lower right) show radiation (red), Coulomb (blue) and total (black) field computed using 200 million particles.





Self-consistent benchmark: Two-body dynamics with retarded Lienard-Wiechert fields

- With the advent of parallel computers in the 1990's, 3D space-charge codes became a reality from the 2000's onward
- But despite progress in space-charge modeling, a key problem that remains – even now in the 2020's – is the 3D simulation of radiative effects
- Lienard-Wiechert (LW) methods provide a natural path from space-charge codes to codes that include both space-charge and radiative phenomena
- The gold standard of classical, particle-based, electrodynamic modeling would be an N-body LW code
- While an N-body LW code with large N is not feasible, a small-N code IS feasible
- Such a code can be used for (1) benchmarking, and (2) shedding light on theories (e.g., Wheeler-Feynman) that can be studied analytically only in special cases

A bit of history drawn from several papers

- D. J. Griffiths, T. C. Proctor, and D. F. Schroeter, Abraham-Lorentz versus Landau-Lifshitz, American Journal of Physics 78, 391 (2010)
- R. D. Driver, Can the Future Influence the Present?, Phys. Rev. D, 19, 4 (1979)
- A. Schild, Electromagnetic Two-Body Problem, Phys. Rev. 131, 6 (1963)
- J. A. Wheeler, R. P. Feynman, Classical Electrodynamics in Terms of Direct Interparticle Action, Reviews of Modern Physics, 21 (3): 425-433, (July 1949)
- J. L. Synge, On the Electromagnetic Two-Body Problem, Proc. of the Royal Society of London, Vol. 177, No. 968 (1940)

What is the correct model for the classical electromagnetic interaction of point particles?

- In 2010 Griffith discussed the self-interaction (radiation reaction) of point particles in classical electrodynamics. He described the difficulties – preacceleration and runaway solutions – in existing treatments like those of Abraham-Lorentz model and Landau-Lifschitz. He wrote,

  This is the skeleton in the closet of classical electrodynamics. Generations of physicists (Dirac, Feynman, and Rohrlich, to name a few) have agonized over the apparent inconsistency. Some have suggested that it presages quantum mechanics; others have argued that it is an artifact of the point limit, indicating that a true point charge is impossible in classical electrodynamics.

Wheeler-Feynman Theory

- In 1949 Wheeler & Feynman wrote “Classical electrodynamics in terms of direct interparticle action.” They said,

  We therefore propose here to go back to the great basic problem of classical physics – the motion of a system of charged particles under the influence of electromagnetic forces…

- They discussed the theory of (*not* instantaneous) action-at-a-distance interaction, and concluded that the theory provides,

  a physically reasonable and experimentally satisfactory account of the classic mechanical behavior of a system of point charges in electromagnetic interaction with one another, free of the ambiguities associated with the idea of a particle acting upon itself.

- Note, however, that Wheeler-Feynman theory involves not only retarded interactions but also *advanced* interactions

The Synge Model

- Prior to Wheeler-Feynman, in 1940 Synge published “On the electromagnetic two-body problem”
- The Synge model includes only retarded interactions
- It predicts that two bound oppositely charged particles will spiral into one another and collide
- It provides an analytic expression (in terms of an integral) for the time to collision
  - This is consistent with our intuitive understanding that accelerating particles must lose energy through radiation, hence they will spiral into one another
- <u>On the other hand</u>, Schild (1963) showed that, in the Wheeler-Feynman model, stationary circular motion <u>is</u> possible

A range of viewpoints

- Synge predicts that bound particles collide
- Wheeler-Feynman predicts bound particles can exhibit circular motion
- Wheeler-Feynman is thought provoking since it uses retarded & advanced LW fields
  - Wheeler-Feynman conclude, on the basis of a thought experiment, that the paradox of future motion affecting present motion is not a paradox after all
  - In "Can the Future Influence the Present?" R.D. Driver shows that, for 1D motion, the differential delay equations can be cast as an initial value problem. That is, in 1D the presence of advanced fields is a property of the mathematical model that can be eliminated by re-expressing the model.
- Wheeler-Feynman has no radiation reaction. But the model starts from a universe of point particles and no "external" fields.
- Other models have radiation reaction. But as Griffiths points out, for finite-sized particles, Abraham-Lorentz and Landau-Lifschitz give different answers. And in the limit of point particles, the equations exhibit preacceleration and runaway solutions.

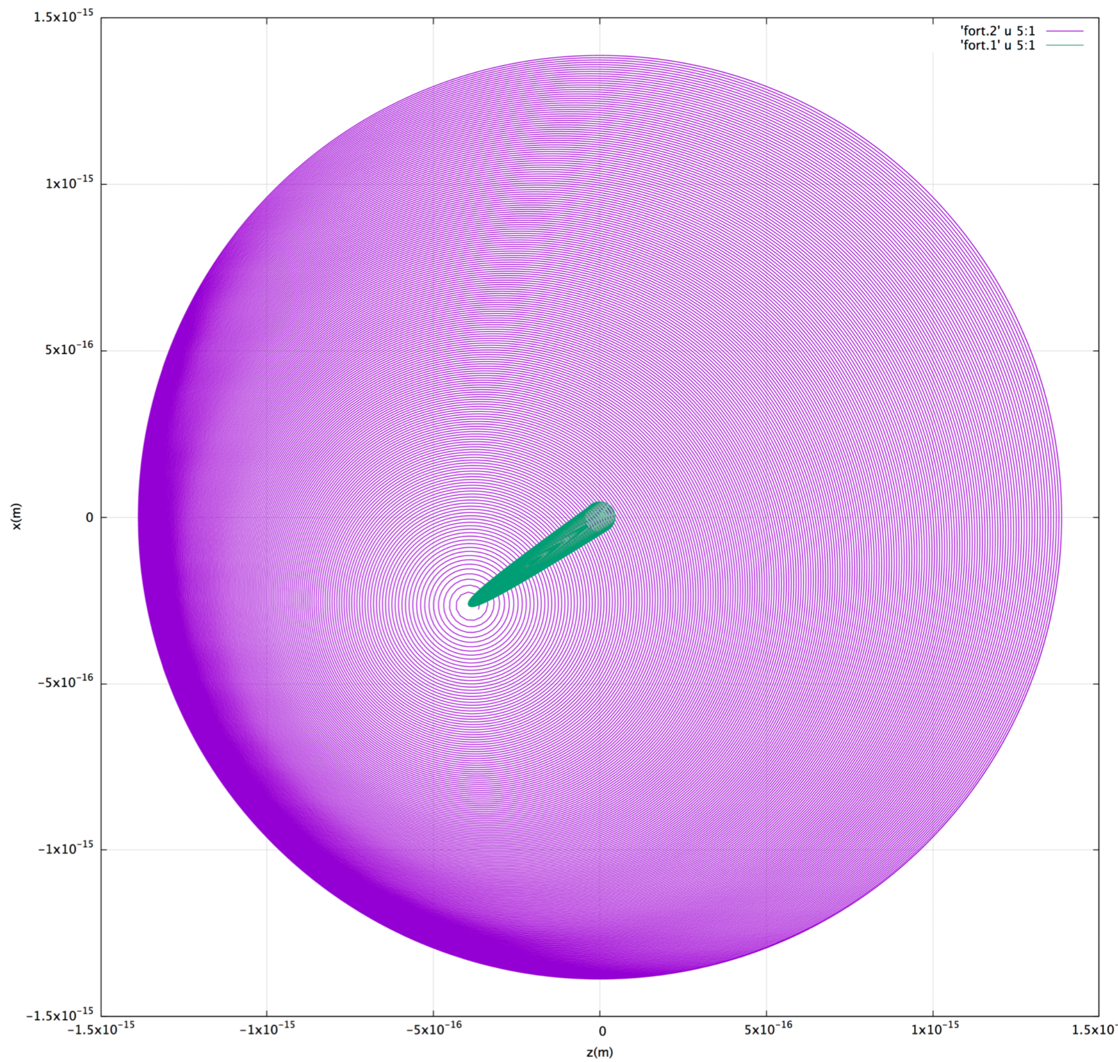
What can we learn from an N-body Lienard-Wiechert code?

- Benchmarking: Regardless of whether the Synge model if physically correct, assuming the analysis is correct it can be used to test a self-consistent LW code based on retarded fields
- Numerical exploration of few-body electrodynamics in various models
- Numerical exploration of the transition from few-body to many-body electrodynamics

Numerical results for the 2-body problem with retarded Lienard-Wiechert fields

The two particles spiraling in toward one another as they radiate and interact via retarded LW fields.

The particles collide in a time in agreement with the analytical calculation of Synge



Status and Conclusions

- Undulator version of the LW3D code is installed on Capulin @ LANL and Cori @ NERSC
- Performance example: A simulation on 9000 cores of Capulin using 1M electrons takes < 5 minutes to compute the LW fields at 20K observation points
- LW3D will be used to test an analytical model of undulator radiation that was developed under the LDRD project
- Work is underway to use LW3D to study self-consistent radiative effects in beam manipulation systems like chicanes
- A self-consistent N-body version of LW3D has been tested on the electrodynamic 2-body problem and exhibits a collision time in agreement with theory

LW3D: Selected publications and presentations

R. Ryne, B. Carlsten, N. Yampolsky, C. Mitchell, J. Qiang, ***Large Scale Simulation of Synchrotron Radiation using a Lienard-Wiechert Approach***, IPAC 2012, New Orleans, http://accelconf.web.cern.ch/accelconf/ipac2012/papers/tuppp036.pdf

R. Ryne, B. Carlsten, N. Yampolsky, C. Mitchell, J. Qiang, ***New Tools for CSR Simulation***, presentation at 2012 Microbunching Workshop, College Park, MD, http://www.umer.umd.edu/events_folder/uBi12/ubi12-Talks/ubi12-Session4/ryne_microbunching_workshop.pdf

R. Ryne, B. Carlsten, N. Yampolsky, C. Mitchell, J. Qiang, ***Massively Parallel Simulation of Radiation Phenomena using a Lienard-Wiechert Approach***, FEL 2013, New York NY, https://accelconf.web.cern.ch/accelconf/FEL2013/talks/moocno04_talk.pdf

B. Garcia, T. Raubenheimer, R. Ryne, **Stochastic Effects from Classical 3D Synchrotron Radiation**, FEL 2017, Santa Fe, NM, http://accelconf.web.cern.ch/AccelConf/fel2017/papers/tup024.pdf

R. Ryne, C. Mitchell, J. Qiang, B. Carlsten, ***Self-Consistent Modeling using a Lienard-Wiechert Particle-Mesh Method***, IPAC 2018, Vancouver, Canada, https://accelconf.web.cern.ch/AccelConf/ipac2018/papers/thpak044.pdf

Collaborators

C. Mitchell, J. Qiang (LBNL)

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N. Yampolsky (LANL)

Acknowledgements

- This research used resources of LANL Institutional Computing including the Capulin HPC system.
- This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.